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The contribution of Fourier analysis in developing functional materials and nanomaterials



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The development of various scientific fields is mainly centred on innovative concepts that are often based on simple ideas, but which are the result of profound reflection. The emergence of '*modern*' physical and chemical approaches and theories such as Relativity, Quantum Mechanics, Radioactivity, Plasma, Chemical Kinetics, Phase Transitions, the design of Molecular Machines, the elaboration of Quantum Dots, etc, would have been impossible without recourse to highly advanced and powerful mathematical concepts and tools. This need had already become apparent over time. For example, in the XIXth century for Electromagnetism and the contribution of partial differential equations; Statistical mechanics, whose founding father can be considered Boltzmann; or in the XXth century with the advent of Quantum Optics and the notion of wave-corpuscle duality to answer the conceptual problem of the nature of light, which has long been a source of debate and divergence within the scientific community.

Despite the fact that the approaches pursued by chemists, physicists and mathematicians are very different in nature, simply as a result of the objectives targeted by each of them, it is nonetheless certain that chemistry, physics and mathematics are intellectual disciplines that are very close, as can be evidenced not only from their history but also from their fruitful exchanges and the enrichment they have brought to one another. In this context, Fourier's analysis and series [1] and their use are the perfect illustration. Indeed, Fourier's contribution has not only revolutionised all areas of scientific research, but it has also undoubtedly had a significant impact on our daily lives (communication and signal processing, analysis techniques, medical imaging, etc.). In this contribution, I will present a few examples and applications [2-3] of the contribution of Fourier series to the development of physicochemical characterisation approaches for functional materials and nanomaterials in the fields of energy transition and renewable energies, digital transition and medicine and pharmacology.

References:

[1] Fourier, J. (1822). *Théorie Analytique de la Chaleur*.

[2] Purtscher, F. R. S., Christianell, L., Rödl, M., Ober, I., Khoder, H., Schwartz, H. A., Bendeif, E-E & Hofer, T.S (2022). Structural Properties of Metal-Organic Frameworks at Elevated Thermal Conditions via a Combined Density Functional Tight Binding Molecular Dynamics (DFTB MD) Approach. *The Journal of Physical Chemistry C*. 127(3)1560-1575.

[3] Ghneim, A., Abou Samra, L., Schaniel, D., Soule, S., Carteret, C & Bendeif, E-E. (2024). *Journal of Non-Crystalline Solids*. Multiscale investigation on the formation path of the apatite phase in bioactive glasses, 639, 123095.